

Discrete-time construction of nonequilibrium path integrals on the Kostantinov-Perel' time contour

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Rigorous nonequilibrium actions for the many-body problem are usually derived by means of path integrals combined with a discrete temporal mesh on the Schwinger-Keldysh time contour. The latter suffers from a fundamental limitation: the initial state on this contour cannot be arbitrary, but necessarily needs to be described by a non-interacting density matrix, while interactions are switched on adiabatically. The Kostantinov-Perel' contour overcomes these and other limitations, allowing generic initial-state preparations. In this Article, we apply the technique of the discrete temporal mesh to rigorously build the nonequilibrium path integral on the Kostantinov-Perel' time contour.

I. INTRODUCTION

The theory of many-body systems brought away from equilibrium strongly relies on the concept of time contours. Introduced in different forms by several authors, including Schwinger¹, Keldysh², and Kostantinov and Perel'³, time contours provide an elegant way to deal on equal footing with time-ordered and anti-time-ordered products of operators which are both needed in the calculation of time-dependent observables out of equilibrium. For appropriately defined time contours, such cumbersome machinery is replaced by a single time-ordering procedure. The price to pay is that the size of the time domain has to be doubled with respect to the physical real-time axis.

Typically, one uses a time contour to evaluate nonequilibrium Green's functions and associated observables. On both the Schwinger-Keldysh and the Kostantinov-Perel' contours, equations of motion can be written down straightforwardly and many-body perturbation theory can be developed in a transparent way^{2,4-6}. In particular, the Kadanoff-Baym equations⁴ are the cornerstone of any numerical calculation of nonequilibrium Green's functions for correlated systems.

Complementary to numerical approaches, path integrals constitute, in the context of nonequilibrium physics, a very useful analytical technique to derive effective theories, kinetic equations, and to derive transparent physical approximations⁷. These integrals are often carried out on the Schwinger-Keldysh (SK) time contour. We here argue that a similarly rigorous derivation for the case of the Kostantinov-Perel' (KP) time contour is timely. Let us first summarize the main features of SK and KP time contours, respectively.

We denote by $\gamma_K = \gamma_{K,+} \cup \gamma_{K,-}$ the SK contour. Here $\gamma_{K,+}$ and $\gamma_{K,-}$ are the forward and backward branches of the real-time axis $(-\infty, +\infty)$, respectively. These are obtained by doubling the real-time degrees of freedom, in the sense that $\gamma_{K,+}$ consists of the real axis traveled forward from $-\infty$ to $+\infty$, while $\gamma_{K,-}$ consists of the real axis traveled backwards from $+\infty$ to $-\infty$. Nonequilibrium theories on the SK contour require to specify the density matrix, $\hat{\rho}_{-\infty}$, which describes the system in the

remote past, i.e. for $t \rightarrow -\infty$. Moreover, this density matrix is required to be non-interacting⁷. Many-body interactions, if present, are switched on adiabatically in such a way that the Hamiltonian coincides with the physical one at a given time $t = t_0$.

The KP contour^{3,6} allows a much greater flexibility with respect to the choice of the initial state of the system. In this formalism, one specifies the preparation of the system at an arbitrary time t_0 ($> -\infty$) via the density matrix $\hat{\rho}_0$, which can always be cast in the form⁶

$$\hat{\rho}_0 \equiv \frac{e^{-\beta \hat{\mathcal{H}}_M}}{\text{Tr}(e^{-\beta \hat{\mathcal{H}}_M})}, \quad (1)$$

where $\beta > 0$ is a positive constant and $\hat{\mathcal{H}}_M$ is an arbitrary Hermitian operator. A standard choice is

$$\hat{\mathcal{H}}_M = \hat{\mathcal{H}}(t_0) - \mu \hat{\mathcal{N}}, \quad (2)$$

where $\hat{\mathcal{H}}(t_0)$ is the physical Hamiltonian of the system at time $t = t_0$, μ is the chemical potential, and $\hat{\mathcal{N}}$ is the number operator. This describes a system at thermal equilibrium at the initial time, in the grand canonical ensemble, with inverse temperature β . However, $\hat{\mathcal{H}}_M$ can be a much more general operator⁶, which allows to select a specific initial state, avoiding to assign the same weight to degenerate eigenstates of the Hamiltonian $\hat{\mathcal{H}}(t_0)$. This allows, for example, to select a broken-symmetry state. Importantly, the KP formulation allows to consider fully interacting systems without resorting to the adiabatic switching on of interactions, and is therefore appropriate for the study of strongly correlated systems. Since the adiabatic switching on is bypassed, one can control the preparation of the system at a finite time t_0 , rather than in the far past.

In this formalism, the real-time domain is $[t_0, \infty)$, and the KP time contour γ is given by the union of three branches: $\gamma = \gamma_+ \cup \gamma_- \cup \gamma_M$. The forward (γ_+) and backward (γ_-) branches are analogous to the SK branches, except that their domain of definition is $[t_0, \infty)$, while the Matsubara branch (γ_M) is the imaginary-time domain needed to describe the initial statistical mixture, $[t_0, t_0 - i\beta)$, where β is the initial inverse temperature

($\hbar = 1$ throughout this Article). One can write Eq. (1) in terms of an evolution operator along the Matsubara branch, i.e.,

$$\hat{\rho}_0 \equiv \frac{\hat{\mathcal{U}}_{\gamma_M}}{\text{Tr}(\hat{\mathcal{U}}_{\gamma_M})}. \quad (3)$$

While the Green's function problem on the KP contour is thoroughly discussed in the literature⁶, a rigorous path-integral formulation seems to be available only in the case of the SK contour⁷. Given the usefulness of path integrals when dealing with problems that can be simplified by field integration, it is convenient to set up the same tools for the KP contour. The problem basically consists in deriving the KP nonequilibrium action, which correctly keeps into account the *boundary terms* arising from the construction of the path integral. This is the goal of the present Article.

Our Article is organized as follows. In Sect. II we introduce a generic time-dependent Hamiltonian, including both fermionic and bosonic degrees of freedom. In Sect. III we present the nonequilibrium partition function and the associated action that we need to derive from “first principles”. In Sect. IV we apply the technique of the discrete temporal mesh to derive the discrete form of the action. In Sect. V we derive the general form of the free-fermion and free-boson Green's functions on the KP contour, which allows to treat boundary conditions exactly while moving to the continuous time representation. We then show several important simplifications that occur in relevant particular cases. In Sect. VI we complete the transition to the continuous-time representation of the action. In Sect. VII we present the solution of a simple nonequilibrium model using both ordinary quantum mechanics and the KP path integral, with the aim of demonstrating the flexibility of the latter in fixing the initial conditions. Finally, in Sect. VIII we summarize our main results and their applicability.

II. HAMILTONIAN

We consider a general system of fermions and bosons described by the following time-dependent Hamiltonian:

$$\hat{\mathcal{H}}(t) \equiv \hat{\mathcal{H}}_f(t) + \hat{\mathcal{H}}_b(t) + \hat{\mathcal{I}}(t). \quad (4)$$

Here,

$$\hat{\mathcal{H}}_f(t) = \hat{d}^\dagger \cdot \mathbf{T}_f(t) \hat{d} \quad (5)$$

is the single-fermion Hamiltonian,

$$\hat{\mathcal{H}}_b(t) = \hat{a}^\dagger \cdot \mathbf{T}_b(t) \hat{a} \quad (6)$$

is the single-boson Hamiltonian, and $\hat{\mathcal{I}}(t)$ includes all the remaining terms. The creation/annihilation operators, \hat{d}^\dagger/\hat{d} for fermions and \hat{a}^\dagger/\hat{a} for bosons, respectively, are grouped into vectors whose components are distinguished

by single-particle quantum numbers (e.g. wavevector and spin projection for electrons on a lattice). We do not make any assumption on the physical nature of the fields that were just introduced. Fermions can be e.g. electrons, holes, or Nambu fermions. Bosons can be e.g. photons or phonons. The term $\hat{\mathcal{I}}(t)$ may include any form of interaction between these fields. The single-particle Hamiltonian matrix $\mathbf{T}_{f/b}(t)$ can include a time-independent hopping (or, if the hopping is diagonalized, the single-particle energy spectrum), as well as the effect of any external time-dependent fields. Setting either $\mathbf{T}_f(t) = 0$ in Eq. (5) or $\mathbf{T}_b(t) = 0$ in Eq. (6) allows us to treat purely bosonic or fermionic systems, respectively.

In the following, we will always use bold fonts to denote matrices in the basis of single-particle quantum numbers.

III. NONEQUILIBRIUM PATH INTEGRALS

We denote the contour variable by $z \in \gamma$. For every real time coordinate $t \in [t_0, \infty)$, there are two values of z : one belonging to γ_+ , which we denote by t_+ , and one belonging to γ_- , which we denote by t_- . A single value of z corresponds to a single imaginary-time coordinate on the Matsubara branch $[t_0, t_0 - i\beta)$.

The nonequilibrium partition function is expressed in terms of an effective action on the KP time contour γ :

$$\begin{aligned} Z[V] &\equiv \frac{\text{Tr}\{\hat{\mathcal{U}}_\gamma^{(V)}\}}{\text{Tr}(\hat{\mathcal{U}}_{\gamma_M})} \\ &\equiv \frac{1}{\text{Tr}(\hat{\mathcal{U}}_{\gamma_M})} \int \mathcal{D}(\bar{d}, d) \int \mathcal{D}(a^*, a) e^{iS^{(V)}[\bar{d}, d; a^*, a]}, \end{aligned} \quad (7)$$

where $\hat{\mathcal{U}}_\gamma^{(V)}$ is the evolution operator along the contour γ , namely $\hat{\mathcal{U}}_\gamma^{(V)} = \hat{\mathcal{U}}_{\gamma_M} \hat{\mathcal{U}}_{\gamma_-}^{(V)} \hat{\mathcal{U}}_{\gamma_+}^{(V)}$ and we have included some source potential $\hat{V}(z)$ depending on the contour variable z . One has $\hat{\mathcal{U}}_\gamma^{(0)} = \hat{\mathcal{U}}_{\gamma_M}$ and therefore $Z[V=0] = 1$. The same identity, i.e. $Z = 1$, applies if $\hat{V}(t_+) = \hat{V}(t_-)$, $\forall t$. For simplicity, we assume that the sources are quadratic in the particle fields. We write the nonequilibrium action as

$$\begin{aligned} S^{(V)}[\bar{d}, d; a^*, a] &\equiv S_{f,Q}^{(V)}[\bar{d}, d] + S_{b,Q}^{(V)}[a^*, a] \\ &\quad + S_I[\bar{d}, d; a^*, a], \end{aligned} \quad (8)$$

where

$$S_{f,Q}^{(V)}[\bar{d}, d] \equiv \int_\gamma dz \left\{ \bar{d}(z) \cdot i \partial_z d(z) - \mathcal{H}_f^{(V)}[\bar{d}(z), d(z); z] \right\} \quad (9)$$

and

$$S_{b,Q}^{(V)}[a^*, a] \equiv \int_\gamma dz \left\{ a^*(z) \cdot i \partial_z a(z) - \mathcal{H}_b^{(V)}[a^*(z), a(z); z] \right\} \quad (10)$$

contain all the terms which are quadratic in the fermion or boson fields, respectively, while

$$S_{\mathcal{I}}[\bar{d}, d; a^*, a] \equiv - \int_{\gamma} dz \mathcal{I}[\bar{d}(z), d(z); a^*(z), a(z); z] \quad (11)$$

includes all the other terms, such as interactions between particles of the same or different kind. It is important to notice that, differently from the case of the SK contour, in the present case we must include the Matsubara branch and account for the fact that the Matsubara Hamiltonian $\hat{\mathcal{H}}_M$, introduced in Eq. (1), is, in general, different from the physical Hamiltonian at the initial time, $\hat{\mathcal{H}}(t_0)$. In general, one has

$$\hat{\mathcal{H}}_M = \hat{\mathcal{H}}(t_0) - \mu_f \hat{\mathcal{N}}_f - \mu_b \hat{\mathcal{N}}_b + \hat{\mathcal{R}}, \quad (12)$$

where $\mu_{f(b)}$ is the chemical potential for the fermion (boson) subsystem, $\hat{\mathcal{N}}_{f(b)}$ is the fermion (boson) number operator, and $\hat{\mathcal{R}}$ includes all the remaining fermionic and bosonic terms. If the equilibrium state is a grand-canonical thermal distribution, then $\hat{\mathcal{R}} = 0$. If, instead, one wants to realize a different equilibrium state⁶, a term $\hat{\mathcal{R}} \neq 0$ is needed.

As in the previous discussion about the physical Hamiltonian, we separate the terms of the Matsubara Hamiltonian which are quadratic in the particle fields from those which are not. The quadratic terms are of the form $\hat{d}^\dagger \cdot \mathbf{T}_f^M \hat{d}$ and $\hat{a}^\dagger \cdot \mathbf{T}_b^M \hat{a}$, where we have introduced the Matsubara hopping matrices $\mathbf{T}_{f/b}^M$. After moving to the path integral formulation, all the terms which are not quadratic are collected into the quantity $\mathcal{I}[\bar{d}(z), d(z); a^*(z), a(z); z]$, introduced in Eq. (11), while the quadratic terms are included into Eqs. (9) and (10), according to the following definitions:

$$\mathcal{H}_f^{(V)}[\bar{d}(z), d(z); z] \equiv \bar{d}(z) \cdot \mathbf{T}_f^{(V)}(z) d(z) \quad (13)$$

and

$$\mathcal{H}_b^{(V)}[a^*(z), a(z); z] \equiv a^*(z) \cdot \mathbf{T}_b^{(V)}(z) a(z), \quad (14)$$

where

$$\begin{aligned} \mathbf{T}_{f/b}^{(V)}(z) &\equiv \Theta(t_{0-}, z) [\mathbf{T}_{f/b}(t) + \mathbf{V}_{f/b}(z)] \\ &+ \Theta(z, t_{0-}) \mathbf{T}_{f/b}^M. \end{aligned} \quad (15)$$

In the above equations, $\Theta(z, t_{0-})$ equals 1 if z lies on the Matsubara branch, and 0 otherwise (t_{0-} is the initial time taken on the backward branch). On the other hand, $\Theta(t_{0-}, z)$ equals 1 if z lies on either γ_+ or γ_- , and 0 otherwise. We have also included the quadratic sources into Eq. (15). Non-quadratic sources, if present, must be included in Eq. (11). To better grasp the structure of Eq. (15), we emphasize that: 1) $\mathbf{T}_{f/b}(t)$ is the physical time-dependent hopping matrix, so it depends on the real time coordinate t and it has the same value

for $z = t_+$ and $z = t_-$; 2) $\mathbf{V}_{f/b}(z)$ is the source matrix, so it is zero on the Matsubara branch, while on the real-time branches it must take different values for the two contour coordinates corresponding to the same physical time, i.e. $\mathbf{V}_{f/b}(t_+) \neq \mathbf{V}_{f/b}(t_-)$, so that $Z[V] \neq 1$; 3) $\mathbf{T}_{f/b}^M$ is constant on the Matsubara branch and vanishes on the real-time branches, being replaced there by $\mathbf{T}_{f/b}(t)$.

Once this issue about the Matsubara Hamiltonian is taken into account, writing down the explicit form of Eq. (11) is formally analogous to what is done in the case of the SK contour⁷. This term therefore presents no difficulties. In this Article, instead, we deal with the derivation of the explicit forms of Eqs. (9) and (10). Indeed, the operator $i\partial_z$ appearing in these equations is a shorthand for something that needs to be defined with great care within a discrete-time formulation. The difference between the KP γ and SK γ_K time contours requires a generalization of the procedure given in Ref. 7, which employs a discrete temporal mesh to properly take into account boundary conditions. With reference to Ref. 7, in our derivation we also include an arbitrary matrix structure of the hopping matrix.

IV. THE KP ACTION

We now proceed to derive the path integral defining the non-equilibrium partition function on the KP time contour for the system introduced before. We initially use the finite interval $[t_0, t_\infty]$ on the real-time axis (with $t_\infty > t_0$) and take the limit $t_\infty \rightarrow +\infty$ at the end of the derivation. This interval is divided into $N - 1$ arbitrarily small sub-intervals of width δt , so that $t_\infty - t_0 = (N - 1)\delta t$. We take the continuum $N \rightarrow \infty$ limit only at the end. We are therefore led to introduce a discrete set of time values:

$$t_j \equiv t_0 + (j - 1)\delta t, \quad j = 1, 2, \dots, N. \quad (16)$$

Note that $t_1 = t_0$ and $t_N = t_\infty$. To each of the physical time values in Eq. (16) we assign *two* distinct contour coordinates, $t_{j,+} \in \gamma_+$ and $t_{j,-} \in \gamma_-$, respectively belonging to the two real-time KP branches.

We then consider the Matsubara branch $[t_0, t_0 - i\beta]$. We split this interval into $M - 1$ infinitesimally small parts, such that $\beta = (M - 1)\delta t$, and we introduce

$$\tau_j = t_0 - i(j - 1)\delta t, \quad j = 1, 2, \dots, M. \quad (17)$$

We give a common name to the full set of discrete contour variables by introducing $2N + M$ contour coordinates z_j defined as

$$\begin{aligned} z_j &= t_{j,+}, \quad j = 1, 2, \dots, N, \\ z_{N+j} &= t_{(N+1-j),-}, \quad j = 1, 2, \dots, N, \\ z_{2N+j} &= \tau_j, \quad j = 1, 2, \dots, M. \end{aligned} \quad (18)$$

To determine the action $S^{(V)}[\bar{d}, d; a^*, a]$ in Eqs. (7) and (8), which is a function of the fermionic (Grassmann)

fields (\bar{d}, d) and the bosonic (complex) fields (a^*, a) , we use a standard procedure that involves the decomposition of the identity operator of the full Hilbert space over fermionic and bosonic coherent states⁷⁻⁹. Denoting by

$a_j, a_j^*, \bar{d}_j, d_j$ the vectors collecting the fields needed to specify the Hamiltonian in the j -th decomposition of the identity, we write

$$\begin{aligned}
\text{Tr} \left\{ \hat{\mathcal{U}}_\gamma^{(V)} \right\} &= \int d[a_0^*, a_0] \int d[\bar{d}_0, d_0] \langle a_0, d_0 | \hat{\mathcal{U}}_\gamma^{(V)} | a_0, -d_0 \rangle e^{-|a_0|^2} e^{-\bar{d}_0 \cdot d_0} \\
&= \int d[a_0^*, a_0] \int d[\bar{d}_0, d_0] \langle a_0, d_0 | \prod_{j=1}^{2N+M-1} \hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} | a_0, -d_0 \rangle e^{-|a_0|^2} e^{-\bar{d}_0 \cdot d_0} \\
&= \int \prod_{j=1}^{2N+M} d[a_j^*, a_j] \int \prod_{j=1}^{2N+M} d[\bar{d}_j, d_j] e^{-\sum_{j=1}^{2N+M} |a_j|^2} e^{-\sum_{j=1}^{2N+M} \bar{d}_j \cdot d_j} \\
&\quad \times \int d[a_0^*, a_0] \int d[\bar{d}_0, d_0] e^{-|a_0|^2} e^{-\bar{d}_0 \cdot d_0} \langle a_0, d_0 | a_{2N+M}, d_{2N+M} \rangle \left(\prod_{j=1}^{2N+M-1} \langle a_{j+1}, d_{j+1} | \hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} | a_j, d_j \rangle \right) \\
&\quad \times \langle a_1, d_1 | a_0, -d_0 \rangle \\
&= \int \prod_{j=1}^{2N+M} d[a_j^*, a_j] \int \prod_{j=1}^{2N+M} d[\bar{d}_j, d_j] e^{-\sum_{j=1}^{2N+M} |a_j|^2} e^{-\sum_{j=1}^{2N+M} \bar{d}_j \cdot d_j} \\
&\quad \times e^{a_1^* \cdot a_{2N+M}} e^{-\bar{d}_1 \cdot d_{2N+M}} \left(\prod_{j=1}^{2N+M-1} \langle a_{j+1}, d_{j+1} | \hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} | a_j, d_j \rangle \right). \tag{19}
\end{aligned}$$

Since $|a_1, d_1\rangle$ depends only on a_1 and d_1 , and not on a_1^* and \bar{d}_1 , we notice that \bar{d}_1 enters the integral in the combination $e^{-\bar{d}_1 \cdot (d_1 + d_{2N+M})}$ only, while a_1^* enters the integral in the combination $e^{-a_1^* \cdot (a_1 - a_{2N+M})}$ only. Using the representations of ordinary and Grassmann δ functions⁸, we then observe that, for any function $f(a_1, d_1)$,

$$\begin{aligned}
&\int d[a_1^*, a_1] e^{-a_1^* \cdot (a_1 - a_{2N+M})} \int d[\bar{d}_1, d_1] e^{-\bar{d}_1 \cdot (d_1 + d_{2N+M})} \\
&\quad \times f(a_1, d_1) \\
&= f(a_{2N+M}, -d_{2N+M}). \tag{20}
\end{aligned}$$

We then obtain

$$\begin{aligned}
\text{Tr} \left\{ \hat{\mathcal{U}}_\gamma^{(V)} \right\} &= \int \prod_{j=2}^{2N+M} d[a_j^*, a_j] \int \prod_{j=2}^{2N+M} d[\bar{d}_j, d_j] \\
&\quad \times e^{-\sum_{j=2}^{2N+M} (|a_j|^2 + \bar{d}_j \cdot d_j)} \\
&\quad \times \left(\prod_{j=2}^{2N+M-1} \langle a_{j+1}, d_{j+1} | \hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} | a_j, d_j \rangle \right) \\
&\quad \times \langle a_2, d_2 | \hat{\mathcal{U}}_{z_1 \rightarrow z_2}^{(V)} | a_{2N+M}, -d_{2N+M} \rangle. \tag{21}
\end{aligned}$$

Taking δt to be infinitesimally small, we have

$$\begin{aligned}
\hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} &\rightarrow \hat{\mathcal{U}}_{+\delta t}^{(V)} \approx e^{-i\delta t [\hat{\mathcal{H}}(t_j) + \hat{V}(t_{j,+})]}, \quad 1 \leq j \leq N-1; \\
\hat{\mathcal{U}}_{z_N \rightarrow z_{N+1}}^{(V)} &= 1; \\
\hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} &\rightarrow \hat{\mathcal{U}}_{-\delta t}^{(V)} \approx e^{i\delta t [\hat{\mathcal{H}}(t_{2N+1-j}) + \hat{V}(t_{2N+1-j,-})]}, \\
&\quad N+1 \leq j \leq 2N-1; \\
\hat{\mathcal{U}}_{z_{2N} \rightarrow z_{2N+1}}^{(V)} &= 1; \\
\hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} &\rightarrow \hat{\mathcal{U}}_{-i\delta t}^{(V)} = e^{-\delta t \hat{\mathcal{H}}_M}, \\
&\quad 2N+1 \leq j \leq 2N+M-1. \tag{22}
\end{aligned}$$

We now introduce $\hat{\mathcal{H}}(z_j)$, $\hat{V}(z_j)$ and δz_j in such a way that

$$\begin{aligned}
\hat{\mathcal{H}}(z_j) &= \hat{\mathcal{H}}(t_j), \quad \hat{V}(z_j) = \hat{V}(t_{j,+}), \quad 1 \leq j \leq N-1; \\
\hat{\mathcal{H}}(z_j) &= \hat{\mathcal{H}}(t_{2N+1-j}), \quad \hat{V}(z_j) = \hat{V}(t_{2N+1-j,-}), \\
&\quad N+1 \leq j \leq 2N-1; \\
\hat{\mathcal{H}}(z_j) &= \hat{\mathcal{H}}_M, \quad \hat{V}(z_j) = 0, \\
&\quad 2N+1 \leq j \leq 2N+M-1; \tag{23}
\end{aligned}$$

and

$$\begin{aligned}
\delta z_j &= \delta t, \quad 1 \leq j \leq N-1; \\
\delta z_N &= 0; \\
\delta z_j &= -\delta t, \quad N+1 \leq j \leq 2N-1; \\
\delta z_{2N} &= 0; \\
\delta z_j &= -i\delta t, \quad 2N+1 \leq j \leq 2N+M-1.
\end{aligned} \tag{24}$$

We then write the contour evolution operator compactly as

$$\hat{\mathcal{U}}_{z_j \rightarrow z_{j+1}}^{(V)} \rightarrow e^{-i\delta z_j [\hat{\mathcal{H}}(z_j) + \hat{V}(z_j)]}, \tag{25}$$

and we obtain

$$\begin{aligned}
&\text{Tr} \left\{ \hat{\mathcal{U}}_{\gamma}^{(V)} \right\} \\
&= \int \prod_{j=2}^{2N+M} d[a_j^*, a_j] \int \prod_{j=2}^{2N+M} d[\bar{d}_j, d_j] \\
&\times \exp \left\{ - \sum_{j=2}^{2N+M} [a_j^* \cdot (a_j - a_{j-1}) + \bar{d}_j \cdot (d_j - d_{j-1})] \right\} \\
&\times \exp \left\{ -i \sum_{j=1}^{2N+M-1} \delta z_j \left\{ \mathcal{H}[\bar{d}_{j+1}, d_j; a_{j+1}^*, a_j; z_j] \right. \right. \\
&\quad \left. \left. + V[\bar{d}_{j+1}, d_j; z_j] \right\} \right\} \Bigg|_{\substack{a_1 = a_{2N+M} \\ d_1 = -d_{2N+M}}}.
\end{aligned} \tag{26}$$

In the continuous-time representation, one formally puts

$$\begin{aligned}
&\sum_{j=2}^{2N+M} [a_j^* \cdot (a_j - a_{j-1}) + \bar{d}_j \cdot (d_j - d_{j-1})] \\
&\equiv \sum_{j=2}^{2N+M} \delta z_{j-1} [a^*(z) \cdot \partial_z a(z) + \bar{d}(z) \cdot \partial_z d(z)] \Big|_{z=z_j},
\end{aligned} \tag{27}$$

obtaining

$$\text{Tr} \left\{ \hat{\mathcal{U}}_{\gamma}^{(V)} \right\} \equiv \int \mathcal{D}(\bar{d}, d) \int \mathcal{D}(a^*, a) e^{iS^{(V)}[\bar{d}, d; a^*, a]}, \tag{28}$$

where the action is given by Eq. (8). The boundary conditions $a_1 = a_{2N+M}$ and $d_1 = -d_{2N+M}$ make the definition of the operator ∂_z on the contour non-trivial. This is where the construction by means of a discrete temporal mesh proves essential.

V. GREEN'S FUNCTIONS FOR THE QUADRATIC PART OF THE ACTION

A. Derivation of the general formula

In the discrete-time representation, the quadratic actions, Eqs. (9) and (10), read as

$$S_{f,Q}^{(V)}[\bar{d}, d] = \sum_{j,j'=2}^{2N+M} \bar{d}_j \cdot \left(\mathbf{G}_{j,j'}^{-1} \right)_{f,Q}^{(V)} d_{j'}, \tag{29}$$

and

$$S_{b,Q}^{(V)}[a^*, a] = \sum_{j,j'=2}^{2N+M} a_j^* \cdot \left(\mathbf{G}_{j,j'}^{-1} \right)_{b,Q}^{(V)} a_{j'}, \tag{30}$$

where the free-fermion and free-boson inverse Green's functions (GFs) are matrices in the discrete-time coordinates (j, j') , as well as in the free-particle indexes. The latter fact is taken into account by using bold symbols for the GFs. Note that we are using the term “free” in the sense of *non-interacting*. As explained above, external fields coupling with the particles are included. Our goal here is to find the direct GFs by inverting these matrices.

In order to lighten the notation, in the following steps we will omit subscripts and superscripts of the GFs, except for those referring to the discrete-time coordinates. To distinguish between bosons and fermions, we introduce the index $\xi = \pm 1$, where the $+$ sign is for bosons and the $-$ sign is for fermions.

The free-particle inverse GF matrices are then written compactly as

$$\begin{aligned}
i\mathbf{G}_{j,j'}^{-1} &= -\delta_{j,j'} \mathbf{1} + (1 - \delta_{j,2}) \delta_{j',j-1} (\mathbf{1} - i\delta z_{j-1} \mathbf{T}_{j-1}) \\
&\quad + \xi \delta_{j,2} \delta_{j',2N+M} (\mathbf{1} - i\delta t \mathbf{T}_1),
\end{aligned} \tag{31}$$

where the dependence of \mathbf{T}_j on the contour coordinate is detailed in Eqs. (13) and (14). The only formal difference between fermions and bosons is in the ξ -dependent term appearing in the second line of Eq. (31), which reflects the different boundary conditions arising from the construction of the path integral.

The matrix in Eq. (31) is invertible, i.e. the left inverse is the same as the right inverse. We have

$$\begin{aligned}
&\sum_{j''} (i\mathbf{G}_{j,j''}^{-1})(-i\mathbf{G}_{j'',j'}^{-1}) = \delta_{j,j'} \\
&\Rightarrow i\mathbf{G}_{j,j'} - (1 - \delta_{j,2}) \mathbf{x}_{j-1} i\mathbf{G}_{j-1,j'} - \xi \delta_{j,2} \mathbf{x}_1 i\mathbf{G}_{2N+M,j'} \\
&\quad = \delta_{j,j'} \mathbf{1},
\end{aligned} \tag{32}$$

where

$$\mathbf{x}_j \equiv \mathbf{1} - i\delta z_j \mathbf{T}_j. \tag{33}$$

To solve Eq. (32), we first introduce the Ansatz

$$i\mathbf{G}_{j,j'} = \delta_{j,j'} \mathbf{1} - \mathbf{X}_{j,j'} \tag{34}$$

in the second line of Eq. (32), finding

$$\begin{aligned} & -\mathbf{X}_{j,j'} + (1 - \delta_{j,2}) \mathbf{x}_{j-1} \mathbf{X}_{j-1,j'} \\ & - (1 - \delta_{j,2}) \delta_{j-1,j'} \mathbf{x}_{j-1} + \xi \delta_{j,2} \mathbf{x}_1 \mathbf{X}_{2N+M,j'} \\ & - \xi \delta_{j,2} \delta_{j',2N+M} \mathbf{x}_1 = \mathbf{0} . \end{aligned} \quad (35)$$

We split the cases $j = 2$ and $j \neq 2$:

$$\begin{aligned} \mathbf{X}_{2,j'} &= \xi \mathbf{x}_1 (\mathbf{X}_{2N+M,j'} - \delta_{j',2N+M} \mathbf{1}) , \\ \mathbf{X}_{j \neq 2,j'} &= \mathbf{x}_{j-1} \mathbf{X}_{j-1,j'} - \delta_{j-1,j'} \mathbf{x}_{j-1} . \end{aligned} \quad (36)$$

The second equation ($j \neq 2$) is solved by iteration: for some $n < j - 1$,

$$\begin{aligned} \mathbf{X}_{j,j'} &= \left(\overrightarrow{\prod_{m=1}^n} \mathbf{x}_{j-m} \right) \mathbf{X}_{j-n,j'} \\ & - \theta_{1 \leq j-j' \leq n} \left(\overrightarrow{\prod_{m=1}^{j-j'}} \mathbf{x}_{j-m} \right) , \quad j > n + 1 , \end{aligned} \quad (37)$$

where θ_p is the discrete step function ($\theta_p = 1$ if p is true, $\theta_p = 0$ if p is false), and we have introduced the contour-anti-ordered product

$$\overrightarrow{\prod_{m=1}^n} \mathbf{f}_m \equiv \mathbf{f}_1 \mathbf{f}_2 \dots \mathbf{f}_{n-1} \mathbf{f}_n , \quad (38)$$

which is accompanied by the contour-ordered product

$$\overleftarrow{\prod_{m=1}^n} \mathbf{f}_m \equiv \mathbf{f}_n \mathbf{f}_{n-1} \dots \mathbf{f}_2 \mathbf{f}_1 . \quad (39)$$

From Eq. (37), we take $n = j - 2$ and, using the first among Eqs. (36), we find

$$\begin{aligned} \mathbf{X}_{j,j'} &= \xi \left(\overleftarrow{\prod_{m=1}^{j-1}} \mathbf{x}_m \right) (\mathbf{X}_{2N+M,j'} - \delta_{j',2N+M} \mathbf{1}) \\ & - \theta_{j' \leq j-1} \left(\overleftarrow{\prod_{m=j'}^{j-1}} \mathbf{x}_m \right) , \quad j > 2 . \end{aligned} \quad (40)$$

We take $j = 2N + M$ and solve for every j' :

$$\begin{aligned} \mathbf{X}_{2N+M,j'} &= -(\mathbf{1} - \xi \mathbf{y}_{2N+M})^{-1} \mathbf{y}_{2N+M} \mathbf{y}_{j'}^{-1} \\ & + \delta_{j',2N+M} \mathbf{1} , \end{aligned} \quad (41)$$

where we have introduced the quantities

$$\mathbf{y}_j \equiv \left(\overleftarrow{\prod_{m=1}^{j-1}} \mathbf{x}_m \right) , \quad \mathbf{y}_j^{-1} = \left(\overrightarrow{\prod_{m=1}^{j-1}} \mathbf{x}_m^{-1} \right) . \quad (42)$$

Inserting Eq. (41) into Eq. (40), we solve the latter for $3 \leq j \leq 2N + M - 1$, while we solve for $j = 2$ using

Eq. (36). The solutions for these cases can be combined into a single one:

$$\mathbf{X}_{j,j'} = \mathbf{y}_j \left[-\xi (\mathbf{1} - \xi \mathbf{y}_{2N+M})^{-1} \mathbf{y}_{2N+M} - \theta_{j' \leq j-1} \mathbf{1} \right] \mathbf{y}_{j'}^{-1} . \quad (43)$$

It can be seen that Eq. (43) coincides with Eq. (41) for $j = 2N + M$. Therefore, Eq. (43) represents the full solution for all values of j, j' . From Eq. (34), we find the free-particle GF:

$$i\mathbf{G}_{j,j'} = \mathbf{y}_j \left[\xi (\mathbf{y}_{2N+M}^{-1} - \xi \mathbf{1})^{-1} + \theta_{j' \leq j} \mathbf{1} \right] \mathbf{y}_{j'}^{-1} . \quad (44)$$

We now take the continuum limit. We first introduce

$$\begin{aligned} t_j &= t_0 + (j - 1)\delta t , \quad \text{if } 1 \leq j \leq N ; \\ t_j &= t_0 + (2N - j)\delta t , \quad \text{if } N + 1 \leq j \leq 2N ; \\ t_j &= t_0 - i(j - 2N - 1)\delta t , \quad \text{if } 2N + 1 \leq j \leq 2N + M . \end{aligned} \quad (45)$$

These identities give the real (if $1 \leq j \leq 2N$) or complex (if $2N + 1 \leq j \leq 2N + M$) time coordinates on the contour corresponding to the discrete index j .

Taking δt as infinitesimally small, we find

$$\mathbf{y}_j \rightarrow \mathcal{T}_\gamma \exp \left[-i \int_{t_{0+}}^{z_j} dz' \mathbf{T}(z') \right] \quad (46)$$

and

$$\mathbf{y}_j^{-1} \rightarrow \overline{\mathcal{T}}_\gamma \exp \left[i \int_{t_{0+}}^{z_j} dz' \mathbf{T}(z') \right] , \quad (47)$$

where \mathcal{T}_γ is the contour-ordering operator along γ , and $\overline{\mathcal{T}}_\gamma$ is the analogous contour-anti-ordering operator. In particular,

$$\begin{aligned} \mathbf{y}_{2N+M}^{-1} &\rightarrow \overline{\mathcal{T}}_\gamma \exp \left[i \int_\gamma dz' \mathbf{T}(z') \right] \\ &= \left\{ \overline{\mathcal{T}}_\gamma \exp \left[i \int_{t_{0+}}^{t_{0-}} dz' \mathbf{T}(z') \right] \right\} \exp(\beta \mathbf{T}^M) , \end{aligned} \quad (48)$$

where the simplification is possible due to the contour structure of the hopping detailed in Eq. (15). In the second step of Eq. (48), the contour-anti-ordered exponential is different from $\mathbf{1}$ only in the presence of sources, while the term $\exp(\beta \mathbf{T}^M)$ is a matrix generalization of the inverse Boltzmann factor. This suggests to introduce a generalized occupation-number matrix,

$$\begin{aligned} \mathbf{n}_\xi &\equiv (\mathbf{y}_{2N+M}^{-1} - \xi \mathbf{1})^{-1} \\ &= \left\{ \overline{\mathcal{T}}_\gamma \exp \left[i \int_{t_{0+}}^{t_{0-}} dz' \mathbf{T}(z') \right] \exp(\beta \mathbf{T}^M) - \xi \mathbf{1} \right\}^{-1} . \end{aligned} \quad (49)$$

We will see that, in the simplest cases, this quantity reduces to the standard occupation number.

We now switch to the full continuum notation for the GF, obtaining

$$i\mathbf{G}_\xi(z, z') = \left\{ \mathcal{T}_\gamma \exp \left[-i \int_{t_{0+}}^z dz'' \mathbf{T}(z'') \right] \right\} \times [\xi \mathbf{n}_\xi + \Theta(z, z') \mathbf{1}] \times \left\{ \overline{\mathcal{T}}_\gamma \exp \left[i \int_{t_{0+}}^{z'} dz'' \mathbf{T}(z'') \right] \right\}, \quad (50)$$

where $\Theta(z, z')$ is the step function on γ , with $\Theta(z, z) = 1$.

Eq. (50) represents the explicit nonequilibrium free-fermion and free-boson GFs on the KP time contour γ , for the most general case of a single-particle Hamiltonian with a non-trivial matrix structure, including time-dependent fields *and* sources. We note that, in the absence of sources ($V = 0$), Eq. (50) reduces to the noninteracting GF derived in Ref. 6 with an entirely different method (equations of motion).

We will now consider several relevant cases in which Eq. (50) can be significantly simplified.

B. GFs in the absence of sources

Most nonequilibrium problems require functional differentiation with respect to the sources, followed by the evaluation of the result at $\mathbf{V}(z) = \mathbf{0}$. Therefore, although nonzero sources are needed to make the path integral meaningful, at some point in the calculation one typically needs to compute the GFs in the absence of sources. In this case, $\mathbf{T}(z) = \mathbf{T}(t)$ if $z \in \gamma_+ \cup \gamma_-$, while $\mathbf{T}(z) = \mathbf{T}^M$ if $z \in \gamma_M$. Eqs. (46)-(47) simplify to

$$\mathbf{y}_j = \mathcal{T} \exp \left[-i \int_{t_0}^{t_j} dt' \mathbf{T}(t') \right] \quad \text{if } z_j \in \gamma_+ \cup \gamma_-, \quad (51)$$

$$\mathbf{y}_j = \exp(-\tau \mathbf{T}^M) \quad \text{if } z_j \in \gamma_M, \quad (52)$$

$$\mathbf{y}_j^{-1} = \overline{\mathcal{T}} \exp \left[i \int_{t_0}^{t_j} dt' \mathbf{T}(t') \right] \quad \text{if } z_j \in \gamma_+ \cup \gamma_-, \quad (53)$$

and

$$\mathbf{y}_j^{-1} = \exp(\tau \mathbf{T}^M) \quad \text{if } z_j \in \gamma_M, \quad (54)$$

where \mathcal{T} and $\overline{\mathcal{T}}$ are the standard time-ordering and anti-time-ordering operators on the real axis, respectively, t_j are the time coordinates defined as in Eqs. (45), and $0 < \tau < \beta$ parametrizes the Matsubara branch as $t_0 - i\tau$. In particular,

$$\mathbf{y}_{2N+M} = \exp(-\beta \mathbf{T}^M). \quad (55)$$

The occupation number matrix introduced in Eq. (49) becomes

$$\mathbf{n}_\xi \equiv \left(e^{\beta \mathbf{T}^M} - \xi \mathbf{1} \right)^{-1}, \quad (56)$$

which is the matrix generalization of the occupation number resulting from either the Bose-Einstein or the Fermi-Dirac statistics. Once z and z' are specified, Eq. (50) is simplified using Eqs. (51)-(54) and (56).

C. GFs in the equilibrium case for a diagonal single-particle Hamiltonian

Let us consider the case of an equilibrium single-particle GF and assume that the single-particle Hamiltonian (and, therefore, the GF as well) is diagonal in the single-particle indexes. It should be noted that treating an equilibrium single-particle GF does not mean that the system must be at equilibrium. It only means that one chooses to exclude the nonequilibrium features from the definition of the single-particle Hamiltonian, i.e. the time-dependent fields are included into Eq. (11), despite being quadratic contributions to the action. Let k be the set of single-particle quantum numbers. For a system of electrons on a lattice, such set would consist of the wavevector and a spin projection.

Including in the Matsubara branch a possibly k -dependent chemical potential term (e.g. a spin-dependent chemical potential for electrons), we find $T_{k,k'}(z) = \delta_{k,k'} \varepsilon_k(z)$, with

$$\varepsilon_k(z) = \varepsilon_k - \mu_k \Theta(z, t_{0-}), \quad (57)$$

and the number matrix reduces to the familiar occupation number,

$$n_{\xi;k} = \frac{1}{e^{\beta(\varepsilon_k - \mu_k)} - \xi}. \quad (58)$$

In this case, the free-particle GF is diagonal, with diagonal components given by

$$G_{\xi;k}(z, z') = -i e^{-i[\varepsilon_k(z)(t-t_0) - \varepsilon_k(z')(t'-t_0)]} \times [\xi n_{\xi;k} + \Theta(z, z')], \quad (59)$$

where t and t' are the (complex) time coordinates corresponding to the contour coordinates z and z' , respectively. Recall that $\xi = \pm 1$ distinguishes between the bosonic and fermionic cases, respectively. Eq. (59) represents the generalization of the results given in Ref. 7 for the SK time contour, to the case of the KP time contour.

To better illustrate the main features of Eq. (59), we explicitly consider the various combinations obtained when the positions of z and z' on the contour are specified.

First, consider the case in which both z and z' belong to the real-time branches (either to γ_+ or to γ_-). In this case, one obtains

$$G_{\xi;k}^>(t, t') = -i e^{-i\varepsilon_k(t-t')} (1 + \xi n_{\xi;k}), \quad (60)$$

if $z > z'$ (on the contour) and

$$G_{\xi;k}^<(t, t') = -\xi i e^{-i\varepsilon_k(t-t')} n_{\xi;k} , \quad (61)$$

if $z < z'$.

These coincide with the standard “greater” and “lesser” nonequilibrium GFs which are also found in the SK formalism⁷.

On the KP contour, one also obtains the other Langreth components⁶. If z belongs to one of the two real-time branches, while z' is on the Matsubara branch,

$$G_{\xi;k}^{\uparrow}(t, t_0 - i\tau) = -\xi i e^{-i\varepsilon_k(t-t_0)} e^{(\varepsilon_k - \mu_k)\tau} n_{\xi;k} . \quad (62)$$

In the opposite case, when z belongs to the Matsubara branch and z' to one of the real-time branches,

$$G_{\xi;k}^{\uparrow}(t_0 - i\tau, t) = -i e^{i\varepsilon_k(t-t_0)} e^{-(\varepsilon_k - \mu_k)\tau} \times [1 + \xi n_{\xi;k}] . \quad (63)$$

Finally, if both z and z' belong to the Matsubara branch,

$$G_{\xi;k}^M(t_0 - i\tau, t_0 - i\tau') = -i e^{-(\varepsilon_k - \mu_k)(\tau - \tau')} \times [\theta(\tau - \tau') + \xi n_{\xi;k}] , \quad (64)$$

where $\theta(\tau - \tau')$ is the ordinary step function.

D. Determinant

In several applications which involve field integration over either the fermionic/bosonic degrees of freedom, it is necessary to know the determinant of $(-i\mathbf{G}_{j,j'}^{-1})$. In general, explicit calculations of this quantity are difficult.

However, in the case when the hopping is diagonal, the calculation can be done easily and directly from Eq. (31). The determinant can be evaluated using the Laplace theorem combined with the fact that the determinant of a triangular matrix is the product of its diagonal elements. The result is independent of M and N being even or odd, implying that it is well defined in the limit $M, N \rightarrow \infty$. We obtain (omitting the single-particle quantum numbers)

$$\det(-iG_{j,j'}^{-1}) = 1 - \xi \prod_{j=1}^{2N+M-1} x_j = 1 - \xi y_{2N+M} \rightarrow 1 - \xi e^{-\beta(\varepsilon - \mu)} . \quad (65)$$

VI. FROM THE DISCRETE TO THE CONTINUUM REPRESENTATION

We now apply the continuum representation for the time domain, in order to make the path-integral construction meaningful. We define the operator

$$\hat{\mathbf{G}}_{\xi}^{-1}(z, z') \equiv \frac{(\mathbf{G}_{\xi}^{-1})_{j,j'}}{\delta z_{j-1} \delta z_{j'-1}} , \quad (66)$$

which satisfies

$$\int_{\gamma} dz' \hat{\mathbf{G}}_{\xi}^{-1}(z, z') \mathbf{G}_{\xi}(z', z'') = \mathbf{1} \delta(z, z'') , \quad (67)$$

where $\mathbf{G}_{\xi}(z', z'')$ is given by Eq. (50) and $\delta(z, z'')$ is the Dirac delta on γ , namely

$$\delta(z, z'') \equiv \frac{\delta_{j,j''}}{\delta z_{j-1}} . \quad (68)$$

In the continuum, Eq. (29) reads as

$$S_{f,Q}[\bar{d}, d] = \int_{\gamma} dz dz' \bar{d}(z) \cdot \hat{\mathbf{G}}_{f,Q}^{-1}(z, z') d(z') , \quad (69)$$

while Eq. (30) reads as

$$S_{b,Q}[a^*, a] = \int_{\gamma} dz dz' a^*(z) \cdot \hat{\mathbf{G}}_{b,Q}^{-1}(z, z') a(z') . \quad (70)$$

The dependence on the sources V is implicit. The inverse GFs appearing in Eqs. (69) and (70) are to be considered as merely symbolic objects. Any calculation (involving, for example, field integration or extremization of the action) must, at some stage, rely on a transformation from the inverse GF to the direct GF in Eq. (50). This encodes the boundary conditions arising from the procedure of construction of the path integral, while being fully well-defined in the continuum limit of the time domain.

VII. AN EXAMPLE: SPIN EVOLUTION IN A TIME-DEPENDENT ZEEMAN FIELD

To show how the KP time contour can be used to specify the initial state in practice, we consider a very simple problem that can be solved analytically with elementary means, allowing for a straightforward comparison of the result with that obtained in the realm of path integrals.

The model involves a single electronic orbital subjected to a time-dependent magnetic field along a certain direction x , which couples to the spin through the Zeeman coupling. We neglect interactions, which would affect the doubly-occupied state. The Hamiltonian is

$$\hat{\mathcal{H}}(t) \equiv B_x(t) \hat{s}_x , \quad (71)$$

where $\hat{s}_x = (\hat{d}_{\uparrow}^{\dagger} \hat{d}_{\downarrow} + \hat{d}_{\downarrow}^{\dagger} \hat{d}_{\uparrow})/2$, and $B_x(t)$ is the magnetic field, in appropriate units. We assume $B_x(t_0) = 0$. Our goal is to compute the time-dependent density matrix

$$\rho_{\sigma,\sigma'}(t) \equiv \langle \hat{\mathcal{U}}(t_0, t) \hat{d}_{\sigma}^{\dagger} \hat{d}_{\sigma'} \hat{\mathcal{U}}(t, t_0) \rangle , \quad (72)$$

from which single-particle observables (particle number and spin components) can be read off.

A. Solution of the problem with ordinary quantum mechanics

We first solve the problem by using ordinary quantum mechanics. The Fock space consists of four states: the vacuum $|0\rangle$, the singly-occupied states $\hat{d}_\sigma^\dagger |0\rangle \equiv |\sigma\rangle$, and the doubly-occupied state $\hat{d}_\uparrow^\dagger \hat{d}_\downarrow^\dagger |0\rangle \equiv |\uparrow\downarrow\rangle$. The evolution operator, satisfying $i \partial_t \hat{U}(t, t_0) = \hat{H}(t) \hat{U}(t, t_0)$ and $\hat{U}(t_0, t_0) = \hat{1}$, is obtained directly as

$$\begin{aligned} \hat{U}(t, t_0) = & |0\rangle \langle 0| + |\uparrow\downarrow\rangle \langle \uparrow\downarrow| \\ & + \{\cos[\theta(t)/2] |\uparrow\rangle - i \sin[\theta(t)/2] |\downarrow\rangle\} \langle \uparrow| \\ & + \{\cos[\theta(t)/2] |\downarrow\rangle - i \sin[\theta(t)/2] |\uparrow\rangle\} \langle \downarrow|, \end{aligned} \quad (73)$$

where

$$\theta(t) \equiv \int_{t_0}^t dt' B_x(t'). \quad (74)$$

The expectation value given in Eq. (72) can be calculated from

$$\rho_{\sigma, \sigma'}(t) \equiv \sum_n W_n \langle n | \hat{U}(t_0, t) \hat{d}_\sigma^\dagger \hat{d}_{\sigma'} \hat{U}(t, t_0) | n \rangle, \quad (75)$$

where W_n is the statistical weight of the Fock state $|n\rangle$. The final result is

$$\begin{aligned} \rho_{\sigma, \sigma'}(t) \equiv & W_{\uparrow\downarrow} \delta_{\sigma, \sigma'} + W_{\uparrow} \begin{pmatrix} \cos^2 \left[\frac{\theta(t)}{2} \right] & -\frac{i}{2} \sin[\theta(t)] \\ \frac{i}{2} \sin[\theta(t)] & \sin^2 \left[\frac{\theta(t)}{2} \right] \end{pmatrix}_{\sigma, \sigma'} \\ & + W_{\downarrow} \begin{pmatrix} \sin^2 \left[\frac{\theta(t)}{2} \right] & \frac{i}{2} \sin[\theta(t)] \\ -\frac{i}{2} \sin[\theta(t)] & \cos^2 \left[\frac{\theta(t)}{2} \right] \end{pmatrix}_{\sigma, \sigma'}. \end{aligned} \quad (76)$$

It is important to notice that the freedom on the choice of the weights W_n allows to prepare the system in a non-trivial initial state and to implement symmetry breaking. For example, if we make the rotationally symmetric choice $W_{\uparrow} = W_{\downarrow}$, we get $\rho_{\sigma, \sigma'}(t) = \delta_{\sigma, \sigma'} (W_{\uparrow\downarrow} + 2W_{\uparrow})$: the density matrix becomes time-independent, encoding only information about the (constant) population of the orbital, as all the spin components are zero. It should be noted that this choice, in more sophisticated cases, is not uncommon at all: it is exactly what one would obtain from a standard thermal mixture, $W_n = e^{-\beta(E_n - \mu N_n)} / Z$. The equality between W_{\uparrow} and W_{\downarrow} comes from the degeneracy of the states $|\uparrow\rangle$ and $|\downarrow\rangle$ with respect to the Hamiltonian $\hat{H}(t_0)$. It is by allowing $W_{\uparrow} \neq W_{\downarrow}$ (hence, deviating from a thermal mixture) that rotational symmetry is broken, the z direction is selected as the one along which the spin is aligned in the initial state, and a non-trivial spin evolution occurs in response to the application of a magnetic field perpendicular to z .

B. Solution of the problem by means of the KP path integral approach

Can we obtain the same result (76) within the KP path integral formulation? In particular, do we have the same freedom on the preparation of the initial state? To see this, let us follow the procedure outlined above. Recalling that $B_x(t_0) = 0$, we take the following Hamiltonian on the Matsubara branch:

$$\hat{\mathcal{H}}_M = -\mu (\hat{n}_{\uparrow} + \hat{n}_{\downarrow}) + \sum_{\sigma} (\sigma \Delta) \hat{n}_{\sigma}, \quad (77)$$

where $\hat{n}_{\sigma} = \hat{d}_{\sigma}^\dagger \hat{d}_{\sigma}$. The inclusion of the second term ($\propto \Delta$) in Eq. (77), which is equivalent to assuming a spin-dependent chemical potential, is the key tool that allows to break rotational symmetry in the initial-state preparation.

The nonequilibrium partition function, from Eq. (7), is

$$Z[V] = \frac{1}{\mathcal{Z}} \int \mathcal{D}(\bar{d}, d) e^{iS^{(V)}[\bar{d}, d]}, \quad (78)$$

where

$$\mathcal{Z} = \text{Tr} \left(e^{-\beta \hat{\mathcal{H}}_M} \right) = 1 + e^{\beta(\mu - \Delta)} + e^{\beta(\mu + \Delta)} + e^{2\beta\mu} \quad (79)$$

is the equilibrium grand-canonical partition function, defined in the usual way, except for the inclusion of the symmetry-breaking term ($\propto \Delta$). Because $Z[0] = 1$, we have

$$\int \mathcal{D}(\bar{d}, d) e^{iS^{(0)}[\bar{d}, d]} = \mathcal{Z}. \quad (80)$$

The action is quadratic, as in Eq. (69). The free-electron GF has the general form given by Eq. (50), with \mathbf{T} being a matrix in spin space only:

$$\begin{aligned} \mathbf{T}(z) = & (\sigma_3 \Delta - \mathbf{1} \mu) \Theta(z, t_{0-}) + \sigma_1 \frac{B_x(t)}{2} \Theta(t_{0-}, z) \\ = & \mathbf{T}^M \Theta(z, t_{0-}) + \mathbf{T}(t) \Theta(t_{0-}, z), \end{aligned} \quad (81)$$

where $\mathbf{1}$ is the 2×2 identity and σ_n are ordinary 2×2 Pauli matrices. The source term in the action is

$$V[\bar{d}(z), d(z); z] \equiv \sum_{\sigma, \sigma'} V_{\sigma, \sigma'}(z) \bar{d}_{\sigma}(z) d_{\sigma'}(z), \quad (82)$$

so that the density matrix is obtained from functional differentiation with respect to the source fields as

$$\rho_{\sigma, \sigma'}(t) = \frac{i}{2} \left\{ \frac{\delta Z[V]}{\delta V_{\sigma, \sigma'}(t_+)} + \frac{\delta Z[V]}{\delta V_{\sigma, \sigma'}(t_-)} \right\} \Big|_{V=0}. \quad (83)$$

Carrying out the path integral in Eq. (78), we obtain

$$Z_0[V] = \frac{\det(-i G^{-1}[V])}{\mathcal{Z}} = \frac{e^{\text{tr} \ln(-i G^{-1}[V])}}{\mathcal{Z}}. \quad (84)$$

The explicit calculation of Eq. (83) requires the following identity:

$$\begin{aligned} \text{tr} \frac{\delta \ln(-i G^{-1}[V])}{\delta V_{\sigma',\sigma}(z)} \Big|_{V=0} &= \text{tr} \left\{ G[0] \frac{\delta(G^{-1}[V])}{\delta V_{\sigma',\sigma}(z)} \Big|_{V=0} \right\} \\ &= -G_{\sigma',\sigma}(z, z+0) \end{aligned} \quad (85)$$

where $V = 0$ is intended in the last line. We finally find

$$\rho_{\sigma,\sigma'}(t) = -iG_{\sigma',\sigma}[t_+, (t+0)_+] \equiv -iG_{\sigma',\sigma}^<(t, t). \quad (86)$$

To calculate the GF, let us consider Eq. (50) specialized to our case. Since the GF needs to be calculated in the absence of sources, we can use the simplifications discussed in Sect. VB. We find

$$\begin{aligned} -i\mathbf{G}^<(t, t) &= \left\{ \mathcal{T} \exp \left[-i \int_{t_0}^t dt' \mathbf{T}(t') \right] \right\} \mathbf{n}_f \\ &\quad \times \left\{ \overline{\mathcal{T}} \exp \left[i \int_{t_0}^t dt' \mathbf{T}(t') \right] \right\} \\ &= \exp \left[-i \frac{\theta(t)}{2} \boldsymbol{\sigma}_1 \right] \mathbf{n}_f \exp \left[i \frac{\theta(t)}{2} \boldsymbol{\sigma}_1 \right], \end{aligned} \quad (87)$$

where we have exploited the fact that $\mathbf{T}(t)$ commutes with itself at different times. The exponentials of the Pauli matrix give the usual result:

$$\exp \left[\pm i \frac{\theta(t)}{2} \boldsymbol{\sigma}_1 \right] = \mathbf{1} \cos \left[\frac{\theta(t)}{2} \right] \pm i \boldsymbol{\sigma}_1 \sin \left[\frac{\theta(t)}{2} \right]. \quad (88)$$

Information about the preparation of the initial state is included into the occupation number matrix:

$$\mathbf{n}_f = [\exp(\beta \mathbf{T}^M) + \mathbf{1}]^{-1} = \begin{pmatrix} \frac{1}{e^{\beta(\Delta-\mu)} + 1} & 0 \\ 0 & \frac{1}{e^{\beta(-\Delta-\mu)} + 1} \end{pmatrix}. \quad (89)$$

Eq. (87) then becomes

$$\begin{aligned} -i\mathbf{G}^<(t, t) &= \frac{1}{e^{\beta(\Delta-\mu)} + 1} \begin{pmatrix} \cos^2 \left[\frac{\theta(t)}{2} \right] & \frac{i}{2} \sin [\theta(t)] \\ -\frac{i}{2} \sin [\theta(t)] & \sin^2 \left[\frac{\theta(t)}{2} \right] \end{pmatrix} \\ &\quad + \frac{1}{e^{\beta(-\Delta-\mu)} + 1} \begin{pmatrix} \sin^2 \left[\frac{\theta(t)}{2} \right] & -\frac{i}{2} \sin [\theta(t)] \\ \frac{i}{2} \sin [\theta(t)] & \cos^2 \left[\frac{\theta(t)}{2} \right] \end{pmatrix}. \end{aligned} \quad (90)$$

Considering the matrix transposition and using Eq. (86), we immediately see that the density matrix $\rho_{\sigma,\sigma'}(t)$ calculated from the path integral on the KP contour has the same form as that computed with ordinary quantum mechanics—see Eq. (76)—with the correspondence

$$W_{\uparrow} = \frac{e^{-\beta(\Delta-\mu)}}{\mathcal{Z}}, \quad W_{\downarrow} = \frac{e^{-\beta(-\Delta-\mu)}}{\mathcal{Z}}, \quad W_{\uparrow\downarrow} = \frac{e^{2\beta\mu}}{\mathcal{Z}}. \quad (91)$$

Note that $\Delta \neq 0$ is essential to realize spin symmetry breaking in our example, i.e. to have $W_{\downarrow} \neq W_{\uparrow}$. Moreover, taking the limit $\Delta \rightarrow +\infty$ allows to prepare the system in the $|\downarrow\rangle$ state (i.e. $W_{\downarrow} = 1, W_{\uparrow} = 0$) and, viceversa, taking the limit $\Delta \rightarrow -\infty$ allows to prepare the system in the $|\uparrow\rangle$ state ($W_{\downarrow} = 0, W_{\uparrow} = 1$).

This simple example illustrates the power of the path integral approach on the KP contour, which gives us the full freedom of defining the Hamiltonian on the Matsubara branch in an arbitrary way.

VIII. SUMMARY AND CONCLUSIONS

In summary, we have presented a discrete temporal procedure for the rigorous construction of the nonequilibrium path integral on the Kostantinov-Perel' time contour. Our main result is the mapping between Eqs. (9) and (10) and Eqs. (69) and (70) via Eq. (50).

Our procedure generalizes the one used for the Schwinger-Keldysh contour⁷, allowing us to include the imaginary-time (Matsubara) branch in addition to the real-time branches. Consequently, path-integral theories on the Kostantinov-Perel' time contour can account, in principle, for arbitrarily correlated initial states and/or statistical mixtures, or particular chosen pure states.

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